Superconductor-insulator transition in Coulomb disorder

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Superconductor-insulator transition driven by the decreasing concentration of electrons n is studied in the case of the disorder potential created by randomly positioned charged impurities. Electrons and Cooper pairs (formed by an non-Coulomb attraction) nonlinearly screen the random potential of impurities. Both electrons and Cooper pairs can be delocalized or localized in the resulting self-consistent potential. The border separating the superconductor and insulator phases in the plane of the concentration of electrons and the length of the Cooper pair is found. For a strong disorder the central segment of this border follows the BEC-BCS crossover line defined for a clean sample.

Superconductor-insulator (SI) transition remains a challenging and controversial subject for more than two decades[1,2,3,4,5,6,7,8,9]. One way how SI transition with the decreasing concentration of electrons n can be envisioned is localization of Cooper pairs in a random potential[1]. This approach is good when Cooper pairs weakly overlap and can be considered as repelling each other point-like bosons, which at small external disorder experience Bose-Einstein condensation (BEC). At large disorder the condensate is fragmented and becomes a Bose insulator. If ξ is the size of the Cooper pair created by an (unspecified here) attractive interaction between electrons the condition of the weak overlap between pairs can be written as $n\xi^3 \ll 1$.

In the opposite case, $n\xi^3 \gg 1$ one may better think about separate electrons, which can be localized or delocalized by disorder. In delocalized state, the same attraction leads to the Bardeen-Cooper-Schrieffer (BCS) superconductivity. Thus, at small enough temperatures the metal-insulator transition with the decreasing concentration of electrons leads to the SI transition in the fermion picture as well. In this case, however, SI transition leads into a Fermi insulator.

The goal of this paper is to study the zero temperature SI transition phase diagram in the plane (ξ,n). We suggest a model in which transition to Bose and Fermi insulator happens at strongly different concentrations. These two segments of the SI border line are connected by the long intermediate segment, where $n\xi^3 = 1$. Here and everywhere in this paper we use the scaling approach in the large parameter introduced below and drop all numerical coefficients.

The line $n\xi^3 = 1$ is called BEC-BCS crossover line and in a clean sample it is not related to any phase transitions[10,11]. We, however, show that in our model a long segment of BEC-BCS crossover line plays the role of SI border line.

One can not meaningfully describe localization of bosons without including their repulsive interaction. Therefore, we include the Coulomb repulsion of Cooper pairs in our theory. In other words, in the boson limit Cooper pairs screen random potential. Similarly, in the BCS limit of almost free electrons, the random potential is screened by electrons. We assume that the disorder itself is of a the Coulomb origin. Namely, we assume that in a three dimensional sample there are randomly distributed positive donors with the concentration N_D and negative acceptors with the concentration N_A, while the concentration of electrons is much smaller than both of them, $n = N_D - N_A \ll N$, where $N = N_D + N_A$ is the total concentration of charged impurities. (This model is similar to a heavily doped strongly compensated semiconductor[12,13]). The Coulomb nature of both disorder potential and interaction between electrons and compact pairs makes understanding of screening very easy.

It is known that on the fermion side of the diagram ($n\xi^3 \gg 1$) even at large concentration of electrons $n \sim N$ all electronic states are localized if $Na^3 \ll 1$, where $a = \kappa\hbar^2/me^2$ is the effective Bohr radius in the sample, κ is its dielectric constant and m is the effective mass. Thus we assume that the sample is heavily doped, $Na^3 \gg 1$. This of course requires a large κ or a small effective mass m leading to large $a \gg a_0$, where a_0 is the lattice constant. In this model the disorder is characterized by the single parameter $Na^3 \gg 1$. This the parameter which is used throughout the paper for scaling estimates. Most

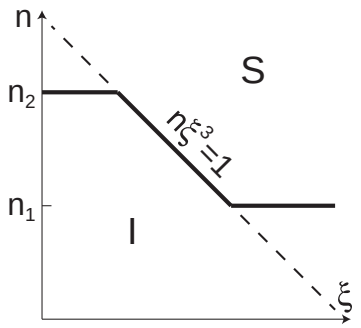

FIG. 1: The phase diagram of the superconductor-insulator transition. On the horizontal axis we plot the length of the pair ξ (in units $N^{-1/3}$) and on vertical line we plot the electron concentration n (in units N) both are in logarithmic scale. S and I stand for the superconductor and insulator. The full line is the border between the superconductor and insulator phases. Its sharp corners are results of schematic nature of this drawing and actually are rounded. The dashed line corresponds to $n\xi^3 = 1$. The lower segments of this line is crossover between Fermi and Bose insulators, the upper one is discussed in the text.

of the theoretical models of the SI transition studied in literature do not have such a parameter and, therefore, have to rely on computer simulations.

An example, where this model may be applicable, is the narrow gap semiconductor PbTe which becomes a superconductor[14] with $T_c \sim 1.5$K, when doping by $\sim 1.5\%$ of Tl ($Pb_{1-x}Tl_xTe$ with $x \sim 0.015$) provides concentrations of holes up to $n \sim 10^{20}$ cm^{-3}. The dielectric constant of PbTe is very large[15], $\kappa > 400$. As a result the Bohr radius a of the Tl acceptor state is so large that no freeze out is observed, i. e. for any studied doping condition of heavy doping $Na^3 \gg 1$ (where N is the concentration of Tl) is fulfilled. It is known that superconductivity of PbTe can be induced only by Tl doping. It is believed[14,16] that Tl is essential for attraction between electrons which happens via quantum valence fluctuations of Tl impurities. One, therefore, can imagine using Tl concentration to tune attraction and, therefore, the pair length ξ, while the concentration of holes n can be tuned by doping with additional donors, which can compensate Tl and make n small enough for SI transition.

Our results are summarized in Fig. 1. The full line shows the SI border. It consists of the two horizontal lines connected by the central segment of the BEC-BCS crossover line $n\xi^3 = 1$. The lower horizontal line

$$n = n_1(N) = \frac{N}{(Na^3)^{1/3}} \ , \tag{1}$$

is the border between the superconductor and the Fermi insulator phases. There is no dependence on ξ here, because electrons are only weakly bound and screen the random potential of charged impurities like free ones. The upper horizontal line

$$n = n_2(N) = \frac{N}{(Na^3)^{1/5}} \tag{2}$$

is the border between the superconductor and Bose insulator phases. Again ξ is irrelevant, because at such small ξ the pairs only weakly overlap and can be considered as point-like bosons. For a given $Na^3 \gg 1$ we have got $n_2(N) \gg n_1(N)$, because bosons have less kinetic energy and one needs more bosons for delocalization (see derivations of $n_1(N)$ and $n_2(N)$ below).

As we mentioned above between the two horizontal lines the SI border follows the BEC-BCS crossover line $n\xi^3 = 1$. Remarkably this part of the border is disorder independent. It exists, however, only for a heavy enough doping, when $Na^3 \gg 1$. At $Na^3 \sim 1$ we would get $n_2(N) \sim n_1(N)$ and the intermediate range, where the border follows $n\xi^3 = 1$, shrinks to zero. We see again how the whole scaling picture rests on the existence of the large parameter $Na^3 \gg 1$.

The origin of the disorder independent intermediate part of the SI border can be understood in the following way. Suppose, we cross this border from below, where we deal with compact Cooper pairs, which are localized by disorder because $n < n_2(N)$. Thus, crossing leads to almost free electrons with the concentration n larger than $n_1(N)$. Electrons with such a concentration are delocalized. Thus, the crossing of the line $n\xi^3 = 1$ leads from the Bose insulator to the superconductor phase. We see that in the presence of a strong disorder the BEC-BCS crossover line gets the new meaning.

Let us make the argument for the intermediate segment of the SI border more formal. We know that the asymptotic segments $n = n_1$ and $n = n_2$ terminate at the line $n\xi^3 = 1$ (the two corners of the border line in Fig. 1). It is natural to assume that between the two termination points there is only one intermediate physical regime or, in other words, these two points are connected by a power law $n(\xi)$ dependence. The only power law connecting these points, is, of course, $n\xi^3 = 1$, i.e. the line of BCS-BEC crossover. Thus, the SI transition border should stick to this line at $n_2 \gg n \gg n_1$.

Let us now derive the concentrations $n_1(N)$ and $n_2(N)$. Actually, the concentration $n_1(N)$ was derived in Ref.[12] as the metal-insulator transition in a heavily doped strongly compensated semiconductor. It was shown also to be in a good agreement with the experimental data for compensated semiconductors[13]. Below we repeat the derivation of $n_1(N)$, because it is a necessary step for our derivation of $n_2(N)$.

Let us divide the sample in cubes with the edge length equal R. Due to spacial fluctuations of the concentrations of donors and acceptor each cube has a random sign charge with the absolute value of the order of $e(NR^3)^{1/2}$. Such randomly alternating charges create the random potential energy relief of the amplitude

$$eV(R) \sim \frac{e^2(NR^3)^{1/2}}{\kappa R} = \frac{e^2(NR)^{1/2}}{\kappa} \ . \tag{3}$$

This energy diverges at large R, so that screening even by a small concentration of electrons n is crucial. To discuss this screening let us estimate the characteristic fluctuating density $\delta N(R)$ of charge for fluctuations with the characteristic scale R. Clearly

$$\delta N(R) = \frac{(NR^3)^{1/2}}{R^3} = \left(\frac{N}{R^3}\right)^{1/2} \ . \tag{4}$$

The concentration n of electrons can be redistributed between wells and hills of the random potential. This redistribution screens all the scales R for which $\delta N(R) = (N/R^3)^{1/2} \leq n$ or, in other words, for $R \geq R_s$, where

$$R_s = \left(\frac{N}{n^2}\right)^{1/3} \tag{5}$$

is the nonlinear screening radius[12,13]. All the scales with $R < R_s$ remain unscreen, because even when all electrons are transferred from all the hills of the potential energy to all its wells they are not able to level off the charge density of such fluctuations. Since $V(R) \propto R^{1/2}$ and thus grows with R, among remaining scales the most important contribution to the random potential is given by

$R = R_s$. Thus, the amplitude of the nonlinearly screened random potential energy is

$$eV(R_s) = \frac{e^2}{\kappa}\frac{N^{2/3}}{n^{1/3}} \ . \tag{6}$$

So far we dealt only with the electrostatic energy of electrons and neglected their kinetic energy. We are talking about the limit of zero temperature, so that all the kinetic energy is of the quantum origin. Now we should find conditions when the quantum kinetic energy is small enough so that described above regime of localized electrons is valid. Clearly the potential energy Eq. (6) is able to localize electrons with concentration n if it is larger than the Fermi energy of electrons $\epsilon_F(n) = \hbar^2 n^{2/3}/2m$ in its wells. In the opposite case $\epsilon_F(n) \gg eV(R_s)$ the Fermi sea covers the typical maxima of the potential energy and the semiconductor behaves as a good metal. Equating $eV(R_s)$ and $\epsilon_F(n)$ we arrive at the critical concentration $n_1(N)$ of the SI transition given by Eq. (1)[12,13].

In the metallic phase electron screening becomes linear, the screening radius is given by the standard Thomas-Fermi expression $R_{TF} = a/(na^3)^{1/6}$ and the amplitude of the screened potential relief is equal $eV(R_{TF}) = e^2(NR_{TF})^{1/2}/\kappa$. These quantities match Eqs. (5) and (6) at $n = n_1$.

Let us now switch to calculation of the critical concentration $n_2(N)$ of electrons in charge $2e$ bosons, corresponding to the SI transition to the Bose insulator. For the insulating phase of localized composite bosons we can exactly repeat the above calculation of the nonlinear screening radius R_s and the random potential energy created by screened charged impurities (6).

The difference between the gas of composite bosons and that of fermions becomes important only at the last step of calculation of the critical concentration, where one has to consider limitations caused by the quantum kinetic energy. Many composite bosons can occupy one localized level of each potential well. Therefore, condition of delocalization of composite bosons is much stronger than the condition $eV(R_s) < \epsilon_F(n)$ used for fermions. Namely, for delocalization of composite bosons we should require that a typical well of the random potential does not have a level, or $eV(R_s) < \hbar^2/mR_s^2$. Solving the equation

$$eV(R_s) = \frac{\hbar^2}{mR_s^2} \ , \tag{7}$$

for n and using Eqs. (6) and (5) we get the critical concentration of the SI transition Eq. (2). This derivation clearly shows why $n_2(N) \gg n_1(N)$. The potential energy amplitude $eV(R_s)$ according to Eq. (6) decreases with increasing n. In order to achieve delocalization in the composite boson case, we had to make $eV(R_s)$ smaller than in the fermion case and this requires the larger concentration $n_2(N) \gg n_1(N)$.

One can arrive at the critical concentration n_2 from the large n superconductor phase of delocalized Cooper pairs, as well. For this purpose we have to start from screening in the case when a composite boson can not be localized inside the well of the size R and in the first approximation its wave function ψ_0 is the plane wave with a very small wave-vector. In the random potential energy with characteristic length R and the amplitude $2eV(R) \ll \hbar^2/mR^2$ this wave function is slightly modulated with the small amplitude $\delta\psi = \psi_0[eV(R)/(\hbar^2/mR^2)]$. For the amplitude of the fluctuating density of charge of electrons with the scale R this gives

$$\delta n(R) = n\frac{eV(R)}{(\hbar^2/mR^2)} \ . \tag{8}$$

All scales R of charge fluctuations for which $\delta n(R) \geq \delta N(R)$ can be screened. Therefore, the equation $\delta n(R) = \delta N(R)$ defines the radius R_d of linear screening by delocalized composite bosons. Using Eqs. (8) and (4) we get

$$R_d = \left(\frac{a}{n}\right)^{1/4} \ . \tag{9}$$

(We could not find this result in the literature.) The meaning of this screening radius is that the Coulomb potential of all fluctuations of charge with $R > R_d$ are screened by small changes of wave functions, while all the fluctuation scales with $R < R_d$ are unscreened. Using Eq. (3) it is easy to see that at $n \gg n_2$ the remaining amplitude of potential energy fluctuations $eV(R_d) \ll \hbar^2/mR_d^2$, so that we indeed deal with delocalized composite bosons. Note that as one should expect the linear screening radius R_d of the delocalized phase matches the nonlinear screening radius R_s of the localized one at $n = n_2$. Of course, simultaneously $V(R_d)$ matches $V(R_s)$.

One can also verify that on the SI border line inequality $R_s \gg \xi$ which we need to consider screening by composite bosons as point like objects fails only at $\xi \sim N^{-1/3}(Na^3)^{2/9}$. This points resides to the right of lower-right corner of SI border line of Fig. 1. This justifies screening calculations presented above.

So far we were concerned with the shape of the full line separating the insulator and superconductor phases on Fig. 1. One may ask whether the two segments of the dashed BEC-BCS crossover line $n\xi^3 = 1$ abandoned by the full line make sense in the insulator phase (the right low corner of the diagram) and in the superconductor phase (the left upper corner). The answer is that these segments of BEC-BCS crossover line imly important crossovers within both phases.

The dashed line in the insulator phase signals the change of a hopping excitation with increasing n from a double charged composite boson to an electron. On both sides of the dashed line the low temperature variable range hopping conductivity obeys the Efros-Shklovskii law[17]

$$\sigma = \sigma_0 \exp\left[-\left(\frac{T_0}{T}\right)^{1/2}\right] \ , \tag{10}$$

but with two different characteristic temperatures T_0. For the large n phase of localized individual electrons (Fermi insulator)

$$T_0 = \frac{Ce^2}{\kappa l} \ , \tag{11}$$

where l is the electron localization length and $C \sim 2.7$[13]. For the low n phase of localized Cooper pairs (Bose insulator) the double charge $2e$ replaces e in Eq. (11). The localization length of a Cooper pair is also smaller than l. Thus, the characteristic temperature T_0 substantially decreases with increasing n or ξ at the BEC-BCS crossover. This leads to the steep increase of the hopping conductivity at the dashed line. This phenomenon is similar to the reduction of the characteristic temperature T_0 by the magnetic field in a granular superconductor discussed recently in Ref.[18].

On the other hand, the dashed line segment in the left upper corner of our phase diagram signals a change in the concentration dependence of the superconductor gap and the critical temperature of the superconductor-metal transition. At this line both quantities start decreasing sharply with the growing n[11].

Above we considered n and ξ as the two independent variables. Strictly speaking this is correct only for $n\xi^3 \leq 1$. Therefore, small ξ (compact bosons) and intermediate segments of the SI border line are found correctly (in the scaling sense). The large ξ segment of our border is above the BEC-BCS crossover line $n\xi^3 = 1$ and, therefore, ξ may be a function of n. (In BCS theory ξ grows with n). This, however, can not affect validity of our result Eq. (1), because the large ξ segment of the border line is not sensitive to ξ at all. This justifies our results for the whole SI border.

Until now we dealt with systems where both impurities and electrons reside in three dimensions (we can call it 3D-3D case). We do not know a 3D-3D system, where n can be made tunable in one sample. More promising can be the 3D-2D case, where impurities residing in three dimensional space (with the three-dimensional concentration N) surround a two-dimensional system of electrons (with the two-dimensional concentration n) and affect it by the Coulomb random potential. This can be a very thin superconductor film on the top of strongly compensated insulator such as a low quality SiO substrate. In such geometry concentration n can be also regulated by a gate[19].

For 3D-2D case one can follow the logic of the calculations above and arrive at a similar phase diagram in the plane (ξ,n). Let us first show the results for this case and then outline the calculation. For the critical concentrations where localization of electrons and composite bosons takes place n_1 and n_2 we arrived at

$$n_1 = \frac{N^{2/3}}{(Na^3)^{1/6}} \ , \qquad n_2 = \frac{N^{2/3}}{(Na^3)^{1/15}} \ , \tag{12}$$

where a is the Bohr radius of two dimensional electrons. The two horizontal segments of the border line $n = n_1$ and $n = n_2$ are connected by the BCS-BEC crossover line $n\xi^2 = 1$, so that the phase diagram in the plane (n, ξ) looks similar to Fig. 1.

The main steps of this calculation are as follows. We again start from from cutting three-dimensional space filled by impurities in cubes with the edge length equal R in such a way that on each side of the plane of the two-dimensional electron gas the first layer of cubes touches the plane. These two first layers create the "projected to the plane" two-dimensional fluctuating charge density of impurities $(NR^3)^{1/2}/R^2$. Equating this density to n we find the nonlinear screening radius $R_s = N/n^2$. Then we calculate the amplitude of the nonlinearly screened random potential energy substituting $R = R_s$ into Eq. (3). This gives

$$eV(R_s) = \frac{e^2}{\kappa}\frac{N}{n} \ . \tag{13}$$

Equating this energy to the Fermi energy $\hbar^2 n/m$ yields n_1, while equating it to $\hbar^2/mR_s^2$ gives n_2. In derivation of Eq. (13) we followed Ref.[20] where similar problem was studied in order to calculate thermodynamic density of states at a small filling factor of a topmost Landau level in quantum Hall effect regime in a MOSFET or a GaAlAs heterostructure without a spacer.

In conclusion, we suggested a model with a strong Coulomb disorder and strong Coulomb interaction, which lets us construct the scaling phase diagram of the SI transition in the plane of the concentration of electrons n and the characteristic length of the Cooper pair ξ both in 3D and 2D systems. The SI border consists of three segments. Two asymptotic segments for a large and small lengths of Cooper pairs describe transitions in the limits of almost free fermions and of compact bosons. They correspond to the two different concentrations of electrons n_1 and n_2. In the strong disorder the threshold concentration for compact Cooper pairs, n_2, is much larger than that for almost free electrons, n_1. As a result for a strong disorder the two asymptotic segments of the border line are connected by the third long segment, which follows the line of BEC-BCS crossover conventionally defined for a clean sample[10,11]. Thus, our model demonstrates that the strong disorder can bring about an important implication for the BEC-BCS crossover line: it becomes the border line of the SI transition.

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